THERMAL PAIRING IN NUCLEI

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Particle-number projection is applied to the modified BCS (MBCS) theory. The resulting approach, called particle-number-projected MBCS theory, taking into account the effects due to fluctuations of particle and quasiparticle numbers at finite temperature, is tested within the exactly solvable multilevel model for pairing as well as the realistic ^{120}Sn nucleus. The results confirm that quasiparticle-number fluctuations indeed smooth out the sharp superfluid-normal phase transition in finite nuclei.

1. Introduction

The BCS and Hartree-Fock-Bogolyubov (HFB) theories use a simple ground-state wave function consisting of a product of Cooper pairs acting on the particle vacuum. Although the pairing problem can be exactly solved [1−3], the simplicity of the BCS and the HFB theories still makes them a preferable choice in the study of finite systems such as atomic nuclei, whose realistic configuration space quite often prevents the feasibility of the exact solutions. However, when the BCS and HFB theories are applied to small systems at finite temperature such as hot nuclei modifications are required because of the large quantal and statistical (thermal) fluctuations, which are ignored in these theories.

Quantal fluctuations (QF) exist within the BCS (HFB) theory even at zero temperature $T = 0$ because of the violation of particle number in the BCS ground-state wave function. To eliminate this deficiency various methods of particle-number projection (PNP) have been proposed, which project out that component of the BCS wave function which corresponds to the right number of particles. The variation after projection (VAP) proposed by Lipkin and Nogami is quite popular as it is computationally simple albeit approximate. The LN equations have non-trivial solutions at any $G \neq 0$, which are quite close to the exact ones when tested in schematic models [4–6].

Statistical fluctuations (SF) in the pairing field have been studied within several approaches based on the Landau's theory of phase transitions [7]. The results of these studies show that the pairing gap does not collapse at the critical temperature T_c as has been predicted by the BCS theory, but decreases monotonously as the temperature increases, and remains finite even at rather high T. The recently proposed modified BCS (MBCS) theory [8,9] and its generation, the modified HFB (MHFB) theory [10], have taken into account the effects due to quasiparticle-number fluctuations (QNF) based on a microscopic foundation. This is realized through a secondary Bogolyubov transformation from quasiparticle operators to modified quasiparticle ones that allows to include the QNF, which is ignored in the conventional BCS and HFB theories at finite temperature, in the generalized single-particle matrix [7]. It has been shown within the MBCS theory [8,9] that it is the QNF that smoothes out the sharp SN phase transition and lead to the non-vanishing thermal pairing in finite systems.

Since the effects of QF are still neglected within the MBCS (MHFB) theory, to give a conclusive answer to the question for SN phase transition in finite systems it is necessary to carry out a PNP in combination with the MBCS (MHFB) theory. In the present paper we will first modify the LN approach by using the secondary Bogolyubov transformation to include the effect of QNF. We also present a second way of combining PNP with the MBCS theory by applying the PAV to the total energy of the system obtained within the MBCS theory to extract the effective thermal gap. These two ways of combining the PNP with the MBCS theory will be called as the modified Lipkin-Nogami (MLN) method [4], and PAV-MBCS theory, respectively. The results of numerical calculations are carried out and analyzed within the exactly solvable equidistant multi-level model called the Richardson model for pairing as well as for the neutron spectrum obtained within the Woods-Saxon potential for ^{120}Sn.

2. Outline of MBCS theory

The MBCS theory includes the quasiparticle-number fluctuations by using the secondary Bogolyubov transformation from quasiparticle operators, $\alpha^{\dagger}_{jm}$ and α_{jm}, to the modified quasiparticle ones, $\bar{\alpha}^{\dagger}_{jm}$ and $\bar{\alpha}_{jm}$, where the indices j and m denote the angular-momentum quantum numbers of single-particle orbitals, while the sign $\tilde{}$ stands for the time-reversal operation, e.g. $a_{j\tilde{m}} = -\mathcal{T}a_{j-m} \equiv (-)^{j-m}a_{j-m}$. By applying successively the original Bogolyubov transformation from particle operators to quasiparticle ones and the secondary Bogolyubov transformation, one obtains a combined transformation between particle and modified quasiparticle operators as

$$a^{\dagger}_{jm} = \bar{u}_j \bar{\alpha}^{\dagger}_{jm} + \bar{v}_j \bar{\alpha}_{j\widetilde{m}} , \quad a_{j\widetilde{m}} = \bar{u}_j \bar{\alpha}_{j\widetilde{m}} - \bar{v}_j \bar{\alpha}^{\dagger}_{jm} , \tag{1}$$

where coefficients $\bar{u}_i$ and $\bar{v}_i$ of the combined transformation (1) are given as

$$\bar{u}_j = u_j \sqrt{1-n_j} + v_j \sqrt{n_j} , \quad \bar{v}_j = v_j \sqrt{1-n_j} - u_j \sqrt{n_j} . \tag{2}$$

Using Eq. (1), one rewrites the pairing Hamiltonian in the modified-quasiparticle representation. Because of the formal Eq. (2) the result has the same form as that of the quasiparticle representation for the pairing Hamiltonian, but with the modified-quasiparticle operators $\bar{\alpha}^{\dagger}_i$, $\bar{\alpha}_i$ replacing the quasiparticle ones $\alpha^{\dagger}_i$, α_i, and coefficients $\bar{u}_i$, $\bar{v}_i$ replacing u_i, v_i. The rest of the derivation is similar to that for the BCS equation. The final result yields the MBCS equation in the form

$$\bar{\Delta} = G \sum_j \Omega_j \bar{\tau}_j , \quad N = 2 \sum_j \Omega_j \bar{\rho}_i , \quad \Omega_j = j + 1/2 , \tag{3}$$

where the modified single-particle density matrix $\bar{\rho}_j$ and modified particle-pairing tensor $\bar{\tau}_j$ are different from the conventional single-particle density matrix ρ_j and particle-pairing tensor τ_j by the terms containing the QNF on j-th orbitals, $\delta\mathcal{N}_j$, namely

$$\bar{\rho}_j = \rho_j - 2u_j v_j \delta\mathcal{N}_j , \quad \bar{\tau}_j = \tau_j - (u_j^2 - v_j^2)\delta\mathcal{N}_j \tag{4}$$

with

$$\rho_j = v_j^2 + (1-2v_j^2) n_j , \quad \tau_j = u_j v_j (1-2n_j) , \quad \delta\mathcal{N}_j = \sqrt{n_j(1-n_j)} . \tag{5}$$

The MBCS internal energy is given as

$$\mathcal{E}_{\rm MBCS} = \sum_j \Omega_j \left[2\epsilon_j \bar{v}_j^2 - G\bar{v}_j^4 \right] - \frac{\bar{\Delta}^2}{G} . \tag{6}$$

The gap and number equations (3) clearly show how the QNF is included within the MBCS theory. This leads to the appearance of the thermal component $\delta\Delta = -G\sum_j \Omega_j (u_j^2 - v_j^2)\delta\mathcal{N}_j$, in addition to the quantal one, $\Delta = G\sum_j \Omega_j \tau_j$, so that $\bar{\Delta} = \Delta + \delta\Delta$. The thermal component $\delta\Delta$ is generated only by QNF in a similar way as that of the phase-fluctuation model, where a gradual projection into a state with exact particle number makes the phases become more and more uncorrelated with increasing temperature. The main feature of each state in the grand canonical ensemble as a coherent superposition of states with different particle numbers is gradually lost so that the BCS-phase ordered regime gradually transforms into a new phase-disordered pseudogap regime. Therefore, we also call the thermal component $\delta\Delta$ of the MBCS gap $\bar{\Delta}$ as the pseudogap.

3. Modified Lipkin-Nogami (MLN) method

The MLN method consists of two self-consistent steps. In the first step, the LN method is applied to remove the particle-number fluctuations inherent in the BCS theory. This leads to a renormalization of the single-particle and quasiparticle energies as

$$\widetilde{\epsilon}_j = \epsilon_j + (4\lambda_2 - G)v_j^2 \ , \qquad \widetilde{E}_j = \sqrt{(\widetilde{\epsilon}_j - \lambda)^2 + \bar{\Delta}^2} \ , \tag{7}$$

where

$$\lambda = \lambda_1 + 2\lambda_2(N+1) \ , \qquad v_j^2 = \frac{1}{2}\left[1 - \frac{\widetilde{\epsilon}_j - \lambda}{\widetilde{E}_j}\right] , \qquad u_j^2 = 1 - v_j^2 \ . \tag{8}$$

In the next step one determines the modified pairing gap $\bar{\Delta}$ and λ from the same MBCS equations (3), where coefficients u_j and v_j from Eq. (8) are used to determine $\bar{u}_j$ and $\bar{v}_j$ in Eq. (2). The coefficient λ_2 is given as

$$\lambda_2 = \frac{G}{4}\frac{\sum_j \Omega_j(1-\bar{\rho}_j)\bar{\tau}_j \sum_{j'} \Omega_{j'}\bar{\rho}_{j'}\bar{\tau}_{j'} - \sum_j \Omega_j(1-\bar{\rho}_j)^2\bar{\rho}_j^2}{\left[\sum_j \Omega_j\bar{\rho}_j(1-\bar{\rho}_j)\right]^2 - \sum_j \Omega_j(1-\bar{\rho}_j)^2\bar{\rho}_j^2} \ . \tag{9}$$

The set of Eqs. (2), (7), (8), and (9) is solved self-consistently, and forms the MLNBCS equations. The total energy is given as

$$\mathcal{E}_{\rm MLN} = \sum_j \Omega_j\left[\epsilon_j - G\bar{\rho}_j\right]\bar{\rho}_j - \frac{\bar{\Delta}^2}{G} - \lambda_2\Delta N^2 \ , \tag{10}$$

where the particle-number fluctuation ΔN^2 is calculated as $\Delta N^2 = 4\sum_j \Omega_j(\bar{u}_j\bar{v}_j)^2$.

4. PAV-MBCS theory

The PNP energy is realized by applying the PNP operator

$$P^N = \frac{1}{2\pi}\int d\phi e^{-i\phi(\hat{N}-N)} \ , \tag{11}$$

on the Hamiltonian whose expectation (average) value in the ground-state (grand canonical ensemble) corresponds to the energy under consideration.

The PNP pairing energy is given as

$$\mathcal{E}^{\rm N}_{\rm pair} = -G\frac{\int d\phi e^{i\phi N}\Big\{\Big[\sum_j \Omega_j \frac{\bar{u}_j\bar{v}_j}{D_j(\phi)}\Big]^2 + \sum_j \Omega_j \frac{\bar{v}_j^4}{D_j(\phi)}\Big\}\det(e^{i\phi})\Big[\det\bar{\mathcal{C}}(\phi)\Big]^{-1/2}}{\int d\phi e^{i\phi N}\Big[\det\bar{\mathcal{C}}(\phi)\Big]^{-1/2}} , \tag{12}$$

where $\bar{\mathcal{C}}(\phi) = e^{2i\phi}/\bar{D}(\phi)$, and $D(\phi) = 1+\bar{\rho}(e^{2i\phi}-1)$. For comparison with the pairing gaps determined within the MBCS theory and MLN method we define an effective gap from the PNP pairing energy as $\Delta_{PNP} = \sqrt{-G\mathcal{E}^{\rm N}_{\rm pair}}$. Notice that the term $-G\sum_j \Omega_j \bar{v}_j^4$ is included in the definition of the effective gap Δ_{PNP}.

5. Numerical analysis

The calculations were carried out within the Richardson model and for ^{120}Sn. The Richardson model consists of Ω doubly-folded equidistant levels, which interact via a pairing force with a constant parameter G. The single-particle energies take the values $\epsilon_j = j\epsilon$ with index j running over all Ω levels. The model is called half-filled when the number Ω of levels is equal to the number N of particles. In general, the number Ω_h of hole levels is not necessary to be the same as the number Ω_p of particle levels, i.e. $\Omega \neq N$. The level distance $\epsilon = 1$ MeV will be used in the present paper. The exact solutions of this model can be found using a number of different methods [1–3]. To use the exact solutions at finite temperature one needs to average them over a statistical ensemble. As the number N of particles in the system is fixed, the canonical ensemble is used here. The only shortcoming of such extension is that, for large N, the exact solutions weighed up to high temperature are impracticable. At the same time, for small N, the small configuration space for the ph-symmetric cases ($\Omega = N$) significantly reduces the limiting temperature up to which the MBCS theory is valid. The reason comes from the symmetry of the QPF profile as a function of single-particle energies with respect to the Fermi level. This profile becomes asymmetric at rather low temperature when $\Omega = N$ is small. It has been demonstrated in [9] that, for $N \leq 14$, its is sufficient to enlarge the space by one more level, $\Omega = N + 1$ to restore the symmetry of the QPF profile up to high temperatures. In the present the predictions within the PNP-MBCS approaches will be compared with the exact solutions for $\Omega = 11$ and $N = 10$. As for the realistic nucleus ^{120}Sn the single-particle energies obtained within the Woods-Saxon potential will be used.

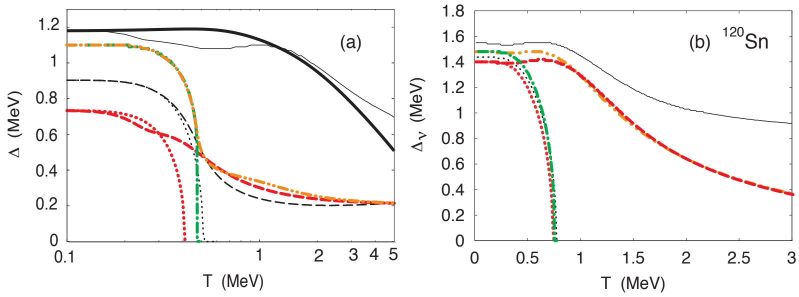

Fig. 1. Pairing gaps as functions of temperature obtained within the Richardson model for ($\Omega = 11$, $N = 10$) (a), and for neutrons in ^{120}Sn (b). The BCS solutions obtained without and including the self-energy term $-Gv_j^2$ in the single-particle energies are shown with the thin and thick dotted lines, respectively. The corresponding MBCS solutions are shown with the thin and thick dashed lines, respectively. The results obtained within the LN and MLN methods are denoted by the dot-dashed and double-dot – dashed lines, respectively. The thin solid line shows the PAV+MBCS effective gap $\Delta_{\rm PNP}$ while the thick solid line in (a) stands for the exact result.

Shown in Fig. 1 are pairing gaps as functions of T. For the Richardson model it is seen in Fig. 1 (a) that, as the particle number is small ($N = 10$), the effect of self-energy term $-Gv_j^2$ in the single-particle energies is rather strong. In the region $T \leq T_{\rm cr}$ the BCS and MBCS gaps obtained including this term are significantly smaller that the values predicted by the BCS and MBCS theories when this term is omitted. The inclusion of the self-energy term also reduces the value of $T_{\rm cr}$ within the BCS theory. At $T \geq 0.7$ MeV the MBCS gap obtained including the self-energy term becomes slightly larger that that obtained ignoring this term. The PNP applied by using the LN method increases the gap at $T = 0$ by nearly 47%. The value of $T_{\rm cr}$ also raises closer to that obtained within the BCS theory ignoring the self-energy term. However, at $T > T_{\rm cr}$ the predictions by the MBCS theory that includes the self-energy term, and by the MLN method are nearly the same, just demonstrating that the quantal fluctuations due to particle-number violation vanish at high temperature. It is also seen that in this region both approaches significantly underestimate the exact result. The situation is largely improved within the PAV-MBCS theory. At $T \leq 0.2$ MeV and 1 MeV $\leq T \leq 2$ MeV the values of the pairing gap predicted by the PAV-MBCS theory almost coincides with the exact one. At 0.2 MeV $\leq T \leq 1$ MeV the PAV-MBCS prediction is slightly lower than the exact result, while at $T > 2$ MeV the discrepancy increases with the PAV-MBCS overestimating the exact result.

The effect of PNP at low T becomes much weaker in ^{120}Sn, where the contribution of the self-energy term is negligible due to the large number of particles. The MBCS and MLN results are close to each other even at low T, while at high T they coalesce. The increasing discrepancy between the PAV-MBCS and MBCS results with increasing T is mainly caused by the $-G\sum_j \Omega_j \bar{v}_j^4$-term, which enters in the definition of the effective gap $G_{\rm PNP}$.

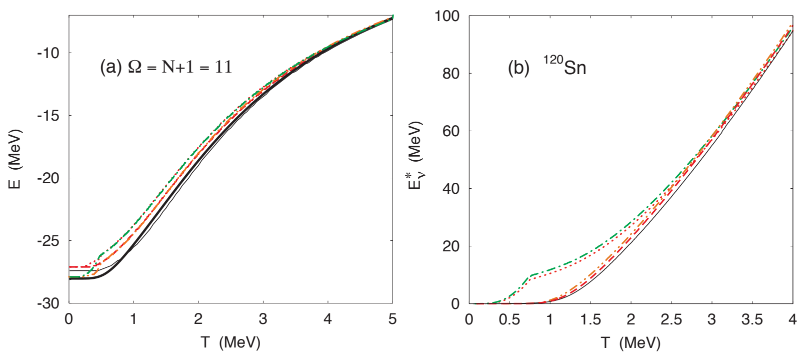

Fig. 2. Total energy (a) and excitation energy (b) as functions of temperature obtained within the Richardson model for ($\Omega = 11$, $N = 10$) (a), and for neutrons in ^{120}Sn (b). Notations are as in Fig. 1

The total energies $\mathcal{E}$ obtained within the approaches under consideration within the Richardson model are plotted as functions of T in Fig. 2 (a). For ^{120}Sn, as the absolute value of the total energy at $T = 0$ is large, we plot in panel (b) of the same figure the excitation energies $E^*_\nu = \mathcal{E}(T) - \mathcal{E}(0)$ for neutrons. It is seen that the QNF indeed smoothes out signature of the sharp SN phase transition from the total and excitation energies even after PNP is taken into account. The effect of PNP is noticeable only at very low temperature, and improves greatly the agreement with the exact result [Fig. 2 (b)]. Increasing the particle number reduces the difference between the MLN, MBCS, and PAV-MBCS, which becomes negligible in ^{120}Sn [Fig. 2 (b)]. As high T all approaches predict nearly the same energy.

The heat capacities calculated as $C = \partial\mathcal{E}/\partial T$ are shown in Fig. 3 as functions of T. It is seen that PNP within the PAV-MBCS smooths out the sharp peak at $T_{\rm cr}$, which is the signature of the SN phase transition, improving greatly the agreement between the PAV-MBCS prediction and the exact result in the schematic case (a).

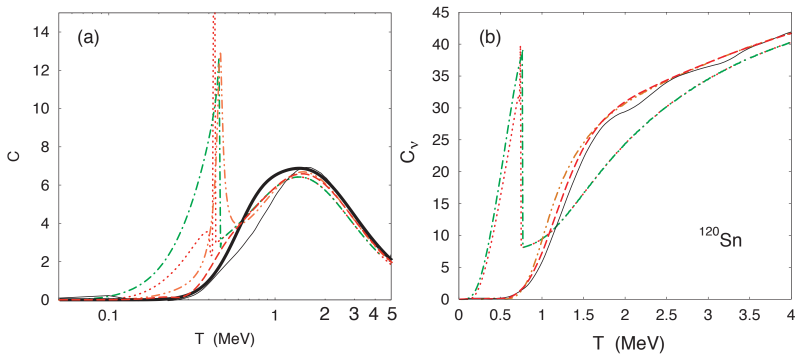

Fig. 3. Heat capacities as functions of temperature within the Richardson model for ($\Omega = 11$, $N = 10$) (a), and for neutrons in ^{120}Sn (b). Notations are as in Fig. 1.

6. Conclusions

This work performs combines the PNP with the MBCS theory. This allows to take into account both quantal and thermal fluctuation effects in the study of SN phase transitions in finite systems such as nuclei. The results in both exactly solvable model and realistic nucleus confirm the previous conclusion by the MBCS theory that thermal fluctuations of quasiparticle number smooths out the sharp SN phase transition in hot nuclei. Therefore, in order to obtain adequate conclusions regarding the superfluid properties of finite systems at finite temperature the approaches based on BCS and HFB theories need to take these thermal fluctuations into account.

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